

MOISTURE DIFFUSION COEFFICIENTS OF SINGLE WHEAT KERNELS WITH ASSUMED SIMPLIFIED GEOMETRIES: ANALYTICAL APPROACH

S. Kang, S. R. Delwiche

ABSTRACT. Using a combination of soaking data and an analytical solution of the diffusion equation, moisture diffusion coefficients of single wheat kernels were determined for nine commercial varieties representing six market classes of U.S. wheat. Two geometric conditions, the whole kernel as a prolate spheroid, and the endosperm (also modeled as prolate spheroidal) and pericarp as separate components, were examined. Values from the analytical solution for a sphere were adjusted by a geometrical correction factor to more closely represent the response of a prolate spheroid. The ranges in diffusion coefficients were 0.39×10^{-10} to 1.04×10^{-10} m²/s for endosperm and 0.04×10^{-10} to 0.28×10^{-10} m²/s for pericarp. Compared to the pericarp, moisture diffused more rapidly in the endosperm. Soft wheats tended to have a more permeable pericarp layer than hard wheats, which resulted in a greater overall rate of diffusion, despite the endosperm of these two groups being nearly equivalent in diffusion coefficient value.

Keywords. Wheat, Moisture, Diffusion, Tempering.

Tempering is an essential step in maximizing flour extraction from wheat kernels. As the pericarp of a wheat kernel absorbs moisture, it toughens which causes fewer small pericarp particles to be released during milling. However, as kernel moisture increases, certain rheological properties change, which may result in a decrease of extracted flour. As part of the effort to achieve an optimal amount of tempering before milling, moisture absorption studies are conducted to understand the distribution and movement of moisture within single kernels of wheat or other small grains.

The diffusion coefficients of various seeds have been determined by using the analytical solution of diffusion equations for different assumed geometries. Hustrulid and Flikke (1959) modified an analytical solution into a simple exponential form and applied it to experimental drying data (~43°C, 10 to 47% RH) of shelled corn. With the kernels assumed to be homogeneous spheres, the exponential form fit the experimental data well. The drying of peanuts in the hull (32 to 43°C, 15 to 68% RH) was described analytically with a finite cylindrical shape assumption (Young and Whitaker, 1971). For peanut kernels (27 to 43°C, 13 to 80% RH), the analytical solution assuming finite or infinite

cylindrical shapes predicted the experiment results with good accuracy (Whitaker and Young, 1972). The infinite cylindrical shape assumption was also used in a moisture diffusion study of heat and mass transfer in rough rice during drying at three temperatures (49, 66, and 82°C) (Husain et al., 1973). The diffusivity of starchy endosperm in white rice during drying (35 to 55°C) was determined using a spherical shape assumption (Steffe and Singh, 1980). Muthukumarappan and Gunasekaran (1990) tested analytical solutions for the adsorption of water vapor (25 to 40°C, 75 to 95% RH) within a corn kernel, assuming the kernel to be an infinite plane sheet, an infinite cylinder or a sphere. Among these assumptions, the infinite sheet model was the best at predicting vapor diffusivity.

Several researchers have investigated moisture diffusion coefficient estimation for individual wheat kernels. Babbitt (1949) obtained a vapor diffusion coefficient and moisture content of whole kernels from adsorption and desorption (drying) experiments, assuming the wheat kernel as a homogeneous sphere. This assumption has been used in other wheat research that involved either drying (Becker and Sallans, 1955, 1956; Jaros et al., 1992) or absorption during soaking (Igathinathane and Chattopadhyay, 1997). Becker (1959) developed general solutions for a wheat kernel of arbitrary shape in the neighborhood of time zero and time infinity. In comparing an analytical solution for a spherical shape and Becker's solution for an arbitrary shape, the importance of the shape effect on the calculated diffusion coefficient was clearly evident. Conversely, on other materials such as tobacco leaf (Walton and Casada, 1986) or a corn kernel (Walton et al., 1988) the shape was determined to be less important than treating the mass as two components (internal and external resistances) rather than one. The solution in the neighborhood of time zero was applied to drying (Becker, 1959) and immersion (Becker, 1960) experiments with wheat kernels. Fan et al. (1961) used Becker's solution for arbitrary shape to calculate diffusion coefficients of several different wheat kernels under various temperature conditions.

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The study of water movement through different regions of the wheat kernel by Hinton (1955) showed that the diffusion rates within the pericarp were lower than other regions including the endosperm. Because of these differences, the diffusivity of endosperm gives little information on the diffusivity of the whole wheat kernel (Glenn and Johnson, 1994). Therefore, diffusion coefficients of endosperm and pericarp in wheat kernels should be determined separately to obtain more accurate information of moisture migration and distribution.

From these studies, it is clear that the analytical solutions based on a proper choice of geometrical shape can predict the absorption, adsorption, and desorption patterns of moisture in single kernels. However, for more accurate estimations of grain moisture diffusion coefficients, certain correction factors (i.e., characteristic length, sphericity) should be further included in the analytical solution, along with consideration of geometrical shape and the use of a two-component (endosperm and pericarp) model, similar to that initially proposed by Walton et al. (1988).

OBJECTIVES

The objective of this research was to better understand the relationship between moisture movement in the wheat kernel and the shape and composition of the kernel. An earlier article (Kang and Delwiche, 1999) described a finite element solution for kernel moisture diffusion. The present article explores the same, but through application of an analytical solution. The specific objectives were to: (1) determine values of diffusion coefficients of the endosperm for different geometrical and physical assumptions; (2) determine values of diffusion coefficients of the pericarp, using the determined values of the endosperm; and (3) compare the result of this two-component model with that of the homogeneous whole kernel model.

ANALYTICAL SOLUTION OF DIFFUSION EQUATION

IDEAL GEOMETRIES OF ONE COMPONENT

The diffusion equation for mass transport within several regular geometric shapes has been analytically solved with the following initial and boundary conditions (Crank, 1975):

1. The initial concentration of moisture is uniform throughout the kernel.
2. At time $t = 0$, the surface moisture content is in equilibrium with the environment, and surface resistance is negligible.
3. For time $t > 0$, the surface is maintained in equilibrium with a constant environment.
4. The moisture content of the kernel approaches equilibrium with the environment at the end of the tempering experiment.

Other assumptions are made for the analytical solutions:

1. The diffusion coefficient of a wheat kernel is constant and not a function of moisture concentration.
2. The kernel is considered isothermal and heat transfer is neglected.

3. The kernel composition is homogeneous and isotropic.
4. The volume change of the kernel is negligible during the tempering process.

Pearled wheat kernels were assumed to have a uniform endosperm. To understand the differences between results using the two-component (endosperm and pericarp) model and the homogeneous model, the diffusion coefficient of a uniform wheat kernel was also determined.

Analytical solutions of the diffusion equation with the above-mentioned conditions can be expressed in terms of the moisture ratio. The general analytical solution for an infinite plane sheet, an infinite cylinder, and a sphere is given as follows (Crank, 1975):

$$MR = \frac{\bar{m}_t - m_{in}}{m_{eq} - m_{in}} = 1 - \sum_{n=1}^{\infty} B_n \exp(-A_n^2 Fo) \quad (1)$$

where

MR = moisture ratio (dimensionless quantity ranging from 0 to 1)

\bar{m}_t = average moisture content at time t (% , dry basis)

m_{eq} = equilibrium moisture content at kernel surface (% , dry basis)

m_{in} = initial moisture content of whole kernel region (% , dry basis)

A_n = constant [= $(2n - 1)(\pi/2)$ for an infinite plane sheet, $r_c \alpha_n$ for an infinite cylinder, and $n\pi$ for a sphere]

B_n = constant (= $2/A_n^2$ for an infinite plane sheet, $4/A_n^2$ for an infinite cylinder, and $6/A_n^2$ for a sphere)

Fo = Fourier number = Dt/L_c^2

D = diffusion coefficient (m^2/s)

t = time variable (s)

L_c = characteristic length (m)

For an infinite plane sheet:

L_c = Volume/Surface area

= l_0

= half-thickness of sheet

For an infinite cylinder:

L_c = $2 \times$ Volume/Surface area

= r_c

= radius of cylinder

For a sphere:

L_c = $3 \times$ Volume/Surface area

= r_s

= radius of sphere

$r_c \alpha_n$ = n th positive root of Bessel function $J_0(r_c \alpha_n) = 0$

$J_0(x)$ = Bessel function of the first kind of order zero

Among analytical solutions for different shapes (infinite plane sheet, infinite cylinder, finite cylinder and sphere), moisture ratio curves (MR vs time) from absorption and desorption experiments have generally matched those from an analytical solution for shapes that resemble the shapes of agricultural products: finite cylinder for the peanuts in the hull (Young and Whitaker, 1971), finite and infinite cylinder for peanut kernels (Whitaker and Young, 1972), infinite cylinder for rough rice kernels (Husain et al., 1973), sphere for white rice (Steffe and Singh, 1980), and infinite plane sheet for corn kernels (Muthukumarappan

and Gunasekaran, 1990). Among these geometries, the shape of a wheat kernel is closest to that of a sphere; hence, an analytical solution for a sphere was chosen as the starting point to be used in determining the diffusion coefficients of whole and pearled wheat kernels.

TWO-COMPONENT SPHERICAL MODEL

It is assumed that the concentration gradient at any point on the surface of endosperm is $\partial C/\partial r$, and the local rate of absorption per unit area is $D_{\text{endosperm}} \partial C/\partial r$, where C is the moisture concentration in a wheat kernel and $D_{\text{endosperm}}$ is the diffusion coefficient of the endosperm. This means that the rate of absorption per unit area of wheat surface is proportional at any time to the difference between the saturated concentration, $C_{\text{saturated}}$, and the actual concentration in the wheat at the interface, C_{surface} . Thus, the surface condition can be written as the following (Danckwerts, 1951):

$$-D_{\text{endosperm}} \partial C/\partial r = (D_{\text{pericarp}}/\delta) \times (C_{\text{surface}} - C_{\text{saturated}}) \quad (2)$$

where $D_{\text{pericarp}}/\delta$ is the proportionality constant, D_{pericarp} is the diffusion coefficient of the pericarp, and δ is the thickness of the pericarp. Moisture ratio can be obtained from the solution for the surface condition (eq. 2), which is (Crank, 1975):

$$MR = 1 - \sum_{n=0}^{\infty} \frac{6Bi^2 \exp(-\beta_n^2 Fo_{\text{endosperm}})}{\beta_n^2 \{\beta_n^2 + Bi(Bi - 1)\}} \quad (3)$$

where

$$\begin{aligned} \beta_n &= \text{the roots of } \beta_n \cot \beta_n + Bi = 1 \\ Bi &= D_{\text{pericarp}} L_c / (D_{\text{endosperm}} \delta) \\ &= \text{mass transfer Biot number} \end{aligned}$$

The Biot number represents the ratio of the internal moisture transfer resistance to the external moisture transfer resistance, which includes the combination of resistances of the pericarp, the pore space (if any) between the endosperm and pericarp, and the external boundary layer, with the latter two resistances considered to be comparatively small (Walton and Casada, 1986; Walton et al., 1988).

The diffusion coefficients of endosperm and pericarp are two unknown variables in equation 3. Values for $D_{\text{endosperm}}$ are determined by application of the one-component model (eq. 1) for pearled wheat, whereupon values for D_{pericarp} are obtained by application of the two component model (eq. 3).

NON-SPHERICAL GEOMETRY CORRECTION

A prolate spheroid is generated by rotating an ellipse about its major axis, known as the polar axis upon rotation. Half the polar axis is the polar radius (c), and the other semi-axis is the equatorial radius (a). Generally, the mean kernel volume calculated from the weight and density of wheat kernels is close to the volume calculated from the equatorial and polar radius of wheat (Becker, 1959). Therefore, radii measurements were used to calculate the

volume of wheat kernels and endosperm. The volume and surface area of a prolate spheroid are:

$$\text{Volume} = 4\pi a^2 c/3 \quad (4)$$

$$\text{Surface area} = 2\pi a \{a + (c/e) \sin^{-1} e\} \quad (5)$$

where

$$\begin{aligned} e &= [(c^2 - a^2)/c^2]^{1/2} \\ &= \text{ellipticity of a prolate spheroid} (= 0 \text{ for a sphere}) \end{aligned}$$

Among the variables in the analytical solution for the sphere, the characteristic length (L_c) and the Fourier number (Fo) provide the method of adjustment of the solution to the prolate spheroid, which is closer than a sphere to the shape of a wheat kernel. The characteristic length is related to shape and size, and reduces to the radius in the case of the sphere. It can be described using the ratio of volume to surface area. The characteristic length for a prolate spheroid is:

$$\begin{aligned} L_c &= 3 \times \text{Volume} / \text{Surface Area} \\ &= 2ac / \{a + (c/e) \sin^{-1} e\} \end{aligned} \quad (6)$$

A sphere with the same volume (V) as a prolate spheroid is said to have an equivalent spherical radius (r_e). For the same moisture ratio curve, the Fourier number of a sphere (Fo_{es}) with equivalent spherical radius is the same as the Fourier number of the prolate spheroid (Fo_{ps}). From the characteristic lengths of the sphere and prolate spheroid, the surface area of a prolate spheroid (S_{ps}) can be described with the characteristic length of a sphere of equal volume (V) and the ratio of the surface area of a sphere of equal volume (S_{es}) to the surface area of the prolate spheroid. Thus, the moisture diffusion coefficient (D_{ps}) of the prolate spheroid can be determined from the relationship between the Fourier number of the sphere and that of the prolate spheroid. The Fourier number of a prolate spheroid is:

$$\begin{aligned} Fo_{\text{ps}} &= D_{\text{ps}} t / (3V/S_{\text{ps}})^2 \\ &= D_{\text{ps}} t / (3V/S_{\text{es}})^2 \times (S_{\text{ps}}/S_{\text{es}})^2 \\ &= [D_{\text{ps}} / (S_{\text{es}}/S_{\text{ps}})^2] t / r_{\text{es}}^2 \\ &= D_{\text{es}} t / r_{\text{es}}^2 = Fo_{\text{es}} \end{aligned} \quad (7)$$

which gives:

$$D_{\text{ps}} = D_{\text{es}} (S_{\text{es}}/S_{\text{ps}})^2 \quad (8)$$

The factor $S_{\text{es}}/S_{\text{ps}}$ is known as sphericity and is the ratio of the surface area of a sphere of equal volume to the surface area of the prolate spheroid.

Equation 1 shows that the moisture ratio depends on the Fourier number. For improved accuracy in determining the diffusion coefficient value, the effect of sphericity and ellipticity of the prolate spheroid shape should be considered. The moisture diffusion coefficient of a wheat kernel is thus determined by using the analytical solution for spherical shape with the characteristic length of a

prolate spheroid. Alternatively, it may be determined by using the analytical solution for a spherical shape, whereupon the value is corrected by the sphericity.

PROCEDURE

WHEAT

Nine wheat varieties, obtained from the USDA Wheat Quality Laboratories at Fargo, North Dakota, Manhattan, Kansas, and Pullman, Washington, were as follows (with wheat class identified in parentheses): Grandin [hard red spring (HRS)], Amidon (HRS), Renville (durum), Jagger [hard red winter (HRW)], TAM107 (HRW), Madsen [soft white winter (SWW)], Rely (club), Penawawa [soft white spring (SWS)], and Vanna (SWS). These varieties represent popular commercial releases grown in the Great Plains or Pacific Northwest regions of the United States. Each variety was represented by one sample. Samples were air-dried, sealed, and kept under refrigeration for 9 to 12 months prior to immersion testing. The sample size of pearled and intact wheat for each variety was 10 to 12 g.

IMMERSION EXPERIMENT

To obtain more uniformly sized kernels, a no. 8 sieve was used to remove broken and small kernels. Twenty grams of each variety was pearled with a Strong Scott pearler (Seedboro Equipment Co., Chicago, Ill.). The lengths along three principal axes were measured for thirty pearled and thirty whole wheat kernels of each sample, and mean values calculated. Half the longest length of the three principal axes was defined as the polar radius, and the mean of the other two half-lengths was defined as the equatorial radius. Table 1 shows the polar radius, equatorial radius and ellipticity of pearled and whole wheats that were used in the immersion experiment. The shape of pearled Renville ($e = 0.86$) was more ellipsoidal than the other varieties. Penawawa ($e = 0.60$) was the closest to being spherical. After pearling, pearled and whole samples were held in a room at 22°C and approximately 65% RH for 72 h. Initial moisture contents of pearled and whole wheat kernels were measured according to the air-oven method for whole grain (130°C, 19 h) following ASAE standard S352.2 (ASAE, 1998).

Table 1. Kernel dimensions (in mm) and ellipticity of pearled and whole wheats*

Variety	Class†	Pearled			Whole		
		Polar Radius	Equatorial Radius	Ellipticity‡	Polar Radius	Equatorial Radius	Ellipticity
Grandin	HRS	2.00	1.53	0.64	2.93	1.59	0.84
Amidon	HRS	2.00	1.40	0.71	3.09	1.48	0.88
Renville	Durum	2.70	1.38	0.86	3.58	1.44	0.92
Jagger	HRW	2.21	1.47	0.75	3.08	1.53	0.87
TAM107	HRW	2.19	1.47	0.74	3.20	1.58	0.87
Madsen	SWW	1.81	1.44	0.61	3.34	1.65	0.87
Rely	Club	1.88	1.31	0.72	3.03	1.39	0.89
Penawawa	SWS	1.71	1.36	0.60	3.12	1.56	0.87
Vanna	SWS	2.10	1.46	0.72	3.23	1.48	0.89

* Means of 30 kernels per variety.

† Hard Red Spring (HRS), Hard Red Winter (HRW), Soft White Winter (SWW), Soft White Spring (SWS).

‡ Ellipticity = $[(c^2 - a^2)/c^2]^{1/2}$, where a and c are the equatorial and polar radii of a prolate spheroid, respectively.

During immersion, room temperature and water temperature were 22°C and room relative humidity was 55% RH. Every fifteen minutes, each sample (ca. 10 g) was taken out of the water bath, blotted on filter paper (Schleicher & Schull Co., No. 588, 18 cm diameter) to remove surface moisture, weighed, and then returned to the bath. The total time for each sample was 240 min (16 × 15 min).

MOISTURE DIFFUSION COEFFICIENT FROM ANALYTICAL SOLUTION

The mean radius, equivalent radius and sphericity of pearled and whole wheat kernels are shown in table 2. Those were used to determine the moisture diffusion coefficient in the analytical solution.

For the two-component model, the diffusion coefficient value of endosperm was determined first from the pearled sample data, and then that of the pericarp, using the result for endosperm. An iteration procedure was used to determine the best moisture diffusion coefficient of the endosperm ($D_{\text{endosperm}}$). The procedure sought the lowest sum of the square of deviations between the experimental moisture ratios of the pearled wheat and the calculated moisture ratios from the analytical solution (eq. 1) at 15-min time increments. The procedure stopped when the difference between moisture diffusion coefficients of successive iterations was less than $10^{-13} \text{ m}^2/\text{s}$. Three different characteristic lengths were used in the analytical solution: (1) the average of two equatorial and one polar radii of wheat; (2) the radius of a sphere that has the same volume as the prolate spheroid; and (3) three times the ratio of volume to surface area of a prolate spheroid (eq. 6).

The diffusion coefficient of pericarp (D_{pericarp}) was determined by the same iteration method and equation 3, based on the determined diffusion coefficient of endosperm. For all samples, the thickness of pericarp was assigned to be 0.125 mm, based on actual measurement of a representative sample.

For the homogeneous model, the diffusion coefficient of whole intact kernel ($D_{\text{whole kernel}}$) was determined using the same iteration method as with the endosperm. The three different characteristic lengths for the analytical solution were determined from the measurements of the whole wheat kernels.

Table 2. Dimensions (in mm) and sphericity of pearled and whole wheat used in the analytical solution procedure

Variety	Pearled			Whole		
	Equivalent			Equivalent		
	Radius*	Radius†	Sphericity	Radius	Radius	Sphericity
Grandin	1.67	1.67	0.99	1.95	1.95	0.94
Amidon	1.57	1.57	0.98	1.89	1.90	0.92
Renville	1.73	1.73	0.93	1.95	1.95	0.89
Jagger	1.68	1.68	0.97	1.93	1.94	0.93
TAM107	1.67	1.68	0.97	1.99	2.00	0.93
Madsen	1.63	1.55	0.99	2.08	2.09	0.93
Rely	1.47	1.48	0.98	1.80	1.80	0.91
Penawawa	1.47	1.47	0.99	1.97	1.97	0.93
Vanna	1.64	1.65	0.98	1.92	1.92	0.91

* Radius = $(2a + c)/3$, where a and c are the equatorial and polar radii of a prolate spheroid, respectively.

† Equivalent radius equals the radius of a sphere that has the same volume as the corresponding prolate spheroid of table 1.

Table 3. Diffusion coefficients of pearled wheat at various geometries at 22°C

Diffusion Coefficient (m ² /s × 10 ¹⁰)				
Variety	Sphere	Sphere at Equivalent Volume of Prolate Spheroid		RMSD(MR)*
		Sphere	Prolate Spheroid	
Grandin	0.62	0.62	0.60	0.0297
Amidon	0.41	0.41	0.39	0.0299
Renville	0.55	0.55	0.48	0.0183
Jagger	0.70	0.70	0.67	0.0414
TAM107	1.09	1.09	1.04	0.0292
Madsen	0.48	0.43	0.42	0.0306
Rely	0.47	0.48	0.46	0.0297
Penawawa	0.44	0.44	0.44	0.0313
Vanna	0.44	0.45	0.43	0.0230
			Ave =	0.0292

* Square root of the mean of the squared differences between the experimental and analytical moisture ratios (eq. 1) calculated at 15-min intervals over the course of a soaking experiment.

RESULTS AND DISCUSSION

DIFFUSION COEFFICIENT OF A PEARLED WHEAT KERNEL

Moisture diffusion coefficients of pearled wheat kernels (endosperm) are shown in table 3. Because the Fourier number is the same for all three shapes, equation 1 will make the root mean square of deviations (RMSD) value the same for all three geometric assumptions. The diffusion coefficient for the prolate spheroid was smaller than that for the sphere. The diffusion coefficient of TAM107 was higher than other varieties, and soft white winter (Madsen) and soft white spring (Penawawa and Vanna) varieties showed similar values. Across all varieties, diffusion coefficient values of the endosperm were within the range of 0.39×10^{-10} to $1.04 \times 10^{-10} \text{ m}^2/\text{s}$.

The moisture diffusion coefficient values of a whole wheat kernel, based on the homogenous model (eq. 1), were within the range of 0.04×10^{-10} to $0.29 \times 10^{-10} \text{ m}^2/\text{s}$ (table 4). The diffusion coefficient values of the pericarp were within the range of 0.04×10^{-10} to $0.28 \times 10^{-10} \text{ m}^2/\text{s}$. The diffusion coefficients of endosperm were larger than those of pericarp, which is in agreement with historical research that concluded that the moisture absorption rate of endosperm is faster than that of pericarp (Hinton, 1955). Unlike other varieties, the diffusion coefficients of the

pericarp of soft white spring varieties, Penawawa and Vanna, were high and each was very close to the three diffusion coefficients listed for the whole kernel. It seems moisture in the pericarp of this class moves faster than in that of other classes. For TAM107, the diffusion coefficients of the whole and the pericarp were also equivalent, albeit very low. Given the high value of diffusion coefficient for endosperm alone, it seems that moisture movement in the whole kernel of TAM107 was greatly restricted by the pericarp. The value for Biot number in table 4 confirms that the moisture transfer resistance in the pericarp of TAM107 is higher than in the endosperm. Biot numbers of soft white winter and spring varieties were higher than those of other classes. The Biot number for mass transfer shows the ratio of the internal mass transfer resistance to the external mass transfer resistance. A Biot number much smaller than 1.0 makes it possible to assume a uniform moisture distribution across a solid at any time during a transient diffusion process, because the external resistance is large compared to the internal resistance. Conversely, a large value of the Biot number implies that the moisture gradients within the solid are significant, i.e., that the moisture difference across the endosperm is much larger than that across the pericarp.

Averaged over all varieties, model accuracy, as defined by the square root of the average sum square of differences between the modeled and analytical moisture ratios, was surprisingly better for the homogeneous model ($\text{RMSD}_{\text{ave}} = 0.0228$) than the two-term model ($\text{RMSD}_{\text{ave}} = 0.0506$, table 4). It appears that only in cases when the Biot number is very low, such as with TAM107 ($\text{Bi} = 0.54$), does accuracy improve with the use of the more complex (i.e., two-component) model (fig. 1). Conversely, the homogeneous model (eq. 1) is more accurate than the two-component model when the pericarp is not as great a barrier to moisture transfer. For example, Penawawa, with a Biot number ($= 9.5$) much larger than one, was more accurately modeled by a homogeneous model ($\text{RMSD} = 0.024$) than by a two-component model ($\text{RMSD} = 0.032$), which tended to underestimate the rate of water penetration (fig. 2).

Table 4. Diffusion coefficients [D ($\text{m}^2/\text{s} \times 10^{10}$)] of whole wheat and pericarp at 22°C

Variety	Whole Kernel (Homogeneous Model)				Pericarp Alone		
	D, Sphere (equivalent volume prolate spheroid)			RMSD (MR)*	D, Prolate Spheroid		Biot No.
	D, Sphere	D, volume prolate spheroid	D, Prolate Spheroid		D†	RMSD (MR)	
Grandin	0.18	0.18	0.16	0.0139	0.12	0.0628	2.85
Amidon	0.17	0.17	0.14	0.0177	0.13	0.0604	4.59
Renville	0.17	0.17	0.13	0.0188	0.11	0.0664	3.06
Jagger	0.19	0.19	0.16	0.0150	0.11	0.0537	2.38
TAM107	0.05	0.05	0.04	0.0439	0.04	0.0153	0.54
Madsen	0.20	0.20	0.17	0.0245	0.15	0.0454	5.55
Rely	0.23	0.23	0.19	0.0274	0.17	0.0660	5.03
Penawawa	0.29	0.29	0.25	0.0240	0.28	0.0325	9.48
Vanna	0.25	0.25	0.21	0.0204	0.22	0.0526	7.13
			Ave =	0.0228	Ave =	0.0506	

* See footnote to table 3.

† The diffusion coefficient refers to that for the pericarp alone; whereas, the RMSD(MR) refers to the whole kernel.

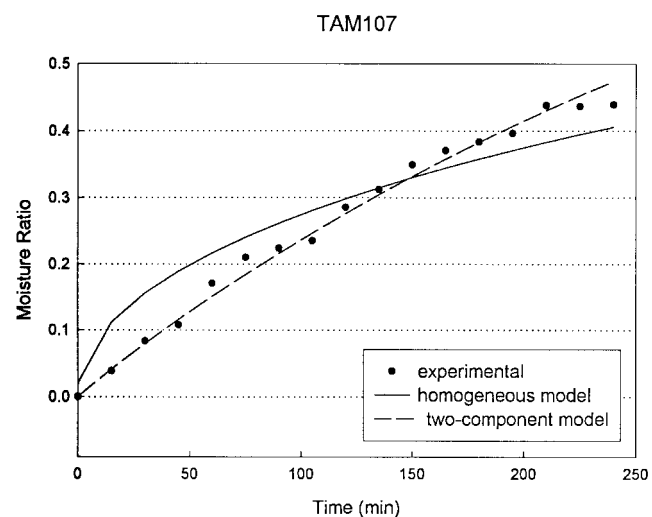


Figure 1—Comparison of moisture ratios determined by soaking (experimental), a one-component (homogeneous) diffusion model, and a two-component diffusion model for the variety 'TAM107'.

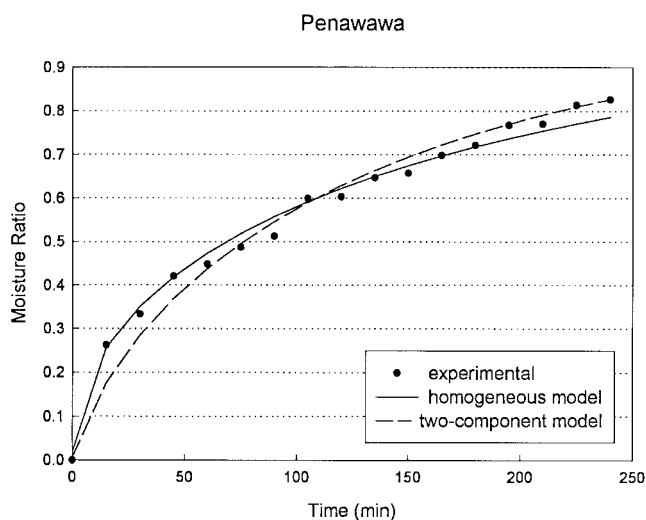


Figure 2—Comparison of moisture ratios determined by soaking (experimental), a one-component (homogeneous) diffusion model, and a two-component diffusion model for the variety 'Penawawa'.

APPLICATION OF GEOMETRICAL CORRECTION TO HISTORICAL DATA

A comparison between the diffusion coefficient from Becker's solution for spherical shape (Becker and Sallans, 1955), Becker's subsequent solution for an arbitrary shape (Becker, 1959), and the present method of applying a prolate spheroid correction factor to a spherical shape solution was conducted. Sphericity was calculated from Becker's wheat data (1959) and used to obtain the diffusion coefficient of wheat based on the analytical solution for a sphere with a prolate spheroid shape correction. Sphericity of Becker's wheat was 0.94 and the determined diffusion coefficient value was close to the diffusion coefficient from Becker's equation for an arbitrary shape (table 5). Because Becker's solution is for the neighborhood of time zero, it is possible to have an error if long-term absorption or desorption data is considered. His equation can be applied to any shape of agricultural products. However, it is not convenient to determine the constant value of the second derivative term in his equation for each experiment.

Table 5. Application of sphericity correction factor to historical published values of diffusion coefficients of whole kernel wheat [cv. Thatcher (HRS)]

Temperature (°C)	Diffusion Coefficient ($\text{m}^2/\text{s} \times 10^{10}$)		
	Historical Values		Sphericity Correction Factor Applied to Spherical Geometry Value‡
	Spherical Geometry*	Arbitrary Geometry†	
24.7	0.097	0.085	0.086
44.3	0.375	0.304	0.333
50.0	0.565	0.432	0.501
52.8	0.635	0.505	0.563
59.4	0.952	0.730	0.845
67.3	1.50	1.13	1.33
79.5	2.77	2.13	2.46

* From Becker and Sallans (1955).

† From Becker (1959).

‡ Sphericity = 0.94, as determined from dimensional values reported in Becker (1959).

Conversely, the analytical solution for idealized geometries of agricultural products, such as wheat, with physical property correction, is easier to use and can reasonably determine moisture diffusion coefficient values.

SUMMARY AND CONCLUSIONS

In this study, the average moisture ratio from immersion data from soaking experiments of whole and pearled (pericarp removed) wheat kernels were related to an analytical solution of diffusion equations for a spherical shape. In the most general form of implementation, the analytical solution of the simplest geometrical shape (e.g., sphere for a wheat kernel) that resembles the agricultural product was selected in the equation for moisture ratio (eq. 1). With use of immersion data to obtain the moisture ratio, this equation was iteratively solved for the diffusion coefficient. For an improved estimate of the moisture diffusion coefficient, the prolate spheroid shape was introduced by using sphericity and ellipticity as geometrical correction factors in the analytical solution for a spherical shape. This procedure was used to determine the diffusion coefficient of wheat endosperm during isothermal moisture tempering. The specific conclusions are as follows:

1. For a wheat kernel, a prolate spheroidal geometry correction factor produces a more accurate estimate of the diffusion coefficient.
2. Low Biot numbers (< 1) favor the use of a two-component (endosperm and pericarp) moisture transfer model.
3. The greater the ellipticity of the wheat kernel, the lower the values of diffusion coefficient become.

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